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1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED			
05 JUN 2014	Final	19-04-2012 to 18-04-2014			
TITLE AND SUBTITLE  Ianipulating Heat Flow through 3 Dimensional Nanoscale Phononic		5a. CONTRACT NUMBER <b>FA23861214047</b>			
Crystal Structure		5b. GRANT NUMBER			
		5c. PROGRAM ELEMENT NUMBER			
6. AUTHOR(S)		5d. PROJECT NUMBER			
Baowen Li		5e. TASK NUMBER			
		5f. WORK UNIT NUMBER			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) National University of Singapore,2 Science Drive 3,Singapore 117542,Singapore,NA,NA		8. PERFORMING ORGANIZATION REPORT NUMBER N/A			
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AOARD, UNIT 45002, APO, AP, 96338-5002		10. SPONSOR/MONITOR'S ACRONYM(S) <b>AOARD</b>			
		11. SPONSOR/MONITOR'S REPORT NUMBER(S) AOARD-124047			
12. DISTRIBUTION/AVAILABILITY STATEMENT  Approved for public release; distribution	on unlimited				
13. SUPPLEMENTARY NOTES					
In this project, we have studied, through computer simulation, how the three dimensional (3D) phononic crystal structures can confine phonon and thus reduce thermal conductivity significantly leading to an enhancement of efficiency of energy conversion in thermoelectric applications. In particular, we have studied a nanoscale 3D Si phononic crystal (PnC) with spherical pores, which can reduce thermal conductivity of bulk Si by a factor up to 10,000 times at room temperature. The phonon participation ratio spectra demonstrate that more phonons are localized as the porosity increases. The thermal conductivity is found insensitive to the temperature changes from room temperature to 1,100K. The effect of period length and mass ratio on thermal conductivity is also studied.					
15. SUBJECT TERMS  phonon transport , Thermoelectric, nano structures, nano photonics					

c. THIS PAGE

unclassified

16. SECURITY CLASSIFICATION OF:

a. REPORT

unclassified

b. ABSTRACT

unclassified

17. LIMITATION OF ABSTRACT

Same as

Report (SAR)

18. NUMBER OF PAGES

1

19a. NAME OF

RESPONSIBLE PERSON

# REPORT DOCUMENTATION PAGE

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OMB No. 0704-0188

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1. REPORT DATE (DD-MM-YYYY) 04-06-2014			3. DATES COVERED (From - To) 19 April 2012 to 18 April 2014	
4. TITLE AND SUBTITLE  Manipulating Heat Flow through 3 Dimensional Nanoscale Phononic Crystal Structure		5a. CONTRACT NUMBER FA23861214047  5b. GRANT NUMBER		
		5c. PR	OGRAM ELEMENT NUMBER	
6. AUTHOR(S)		5d. PR	5d. PROJECT NUMBER	
Prof. Baowen Li		5e. TASK NUMBER		
		5f. WO	RK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAM National University of Sin 2 Science Drive 3 Singapore 117542 Singapore			8. PERFORMING ORGANIZATION REPORT NUMBER  N/A	
9. SPONSORING/MONITORING AGENO	CY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S)	
AOARD UNIT 45002 APO AP 96338-5002			AOARD  11. SPONSOR/MONITOR'S REPORT NUMBER(S)  AOARD-124047	
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16. SECURITY CLASSIFICATION OF:		17. LIMITATION OF	18. NUMBER	19a. NAME OF RESPONSIBLE PERSON	
a. REPORT	b. ABSTRACT	c. THIS PAGE	ABSTRACT	OF PAGES	Tammy Low, Lt Col, USAF, Ph.D.
U	U	U	υυ	1	19b. TELEPHONE NUMBER (Include area code) +81-3-5410-4409

### Final Report for AOARD Grant 124047

# "Manipulating heat flow through three dimensional (3D) nanoscale phononic crystal structure"

Date: June 2, 2014

#### Name of Principal Investigators (PI): Baowen Li

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**Period of Performance**: 04/19/2012 – 04/18/2014

#### Abstract:

In this project, we have studied, through computer simulation, how the three dimensional (3D) phononic crystal structures can confine phonon and thus reduce thermal conductivity significantly leading to an enhancement of efficiency of energy conversion in thermoelectric applications. In particular, we have studied a nanoscale 3D Si phononic crystal (PnC) with spherical pores, which can reduce thermal conductivity of bulk Si by a factor up to 10,000 times at room temperature. The phonon participation ratio spectra demonstrate that more phonons are localized as the porosity increases. The thermal conductivity is found insensitive to the temperature changes from room temperature to 1,100K. The effect of period length and mass ratio on thermal conductivity is also studied.

# Details of the main project can be found in the publication:

L-N Yang, N Yang, and B Li, Extreme Low Thermal Conductivity in Nanoscale 3D Si Phononic Crystal with Spherical Pores, *Nano Letters* **14**, 1734 Published on 21 Feb (2014). dx.doi.org/10.1021/nl403750s

# List of Publications and Significant Collaborations that resulted from your AOARD supported project:

- a. Two papers have been published in peer-reviewed journals,
  - L-N Yang, N Yang, and B Li, Extreme Low Thermal Conductivity in Nanoscale 3D Si Phononic Crystal with Spherical Pores, *Nano Letters* 14, 1734 Published on 21 Feb (2014). dx.doi.org/10.1021/nl403750s
  - 2. L-N Yang, N Yang, and B Li, Reduction of Thermal Conductivity by Nanoscale 3D Phononic Crystal, *Scientific Report* **3**, 1143, published on 31 January 2013
- b. Manuscript submitted but not yet published

L-N Yang, J Chen, N Yang, and B Li, Manipulating Graphene Thermal Conductivity by Phononic

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